GAS PHASE CONFORMATIONAL DISTRIBUTIONS FOR THE 2-ALKYLALCOHOLS 2-PENTANOL AND 2-HEXANOL FROM MICROWAVE SPECTROSCOPY

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Chirped-pulse and cavity Fourier-transform microwave spectrometers were used to record rotational spectra arising from four conformational structures of 2-pentanol and 14 conformations of 2-hexanol. The microwave spectra of these alkylalcohols are very congested because each conformer's rotational spectrum consists of 10 to 89 transitions. Assignments of the spectra to conformational structures were made by comparison of the experimental moments of inertia and dipole-selection-rule intensities to predictions from ab initio (MP2/6-311++G**) model structures. Twenty-seven gauche/anti configurations were found from the optimizations of 2-pentanol, and the 81 starting structures of 2-hexanol converged to 75 unique conformations. The all-anti configurations of 2-pentanol and 2-hexanol were calculated to have the lowest energies and gave rise to the most intense signals. Spectra were assigned to conformers up to 4 kJ mol^{-1} above the minimum energy structures.